MCNP Progress for Nuclear Criticality Safety

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Monte Carlo Codes, XCP-3

Los Alamos National Laboratory

US DOE/NNSA Nuclear Criticality Safety Program –

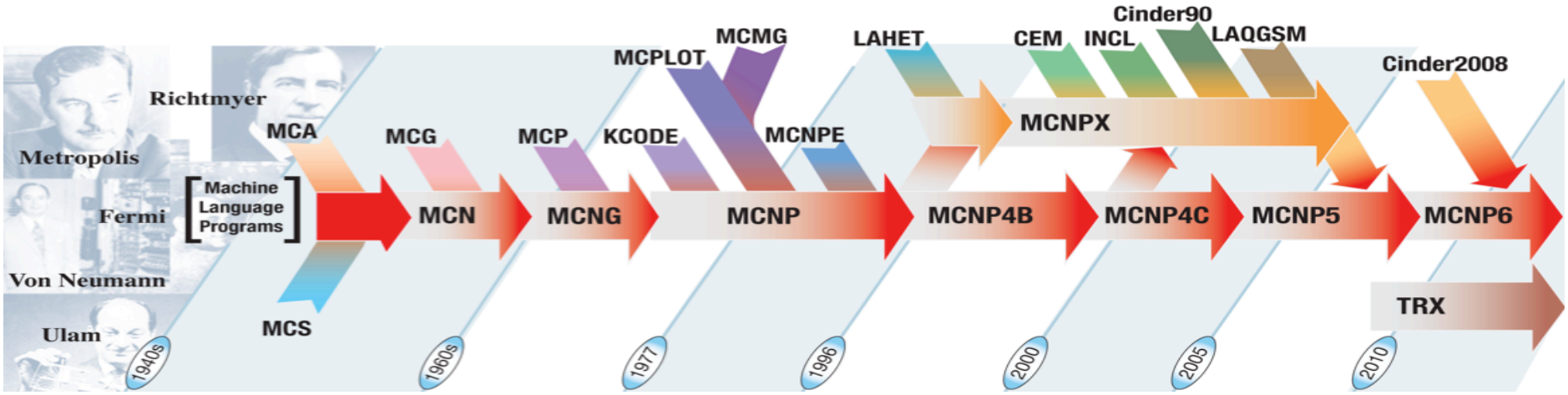
What have we done for you lately ?

- MCNP Release Status
- Verification / Validation
- User Support & Training
- Criticality Related MCNP Development
- Sensitivity and Uncertainty Progress
- Future of MCNP

MCNP Release Status

MCNP6.1 -- The Next Version

Monte Carlo Codes
XCP-3, LANL



- **MCNP release package to RSICC in June 2013**

  MCNP6.1 + MCNP5-1.60 + MCNPX-2.70

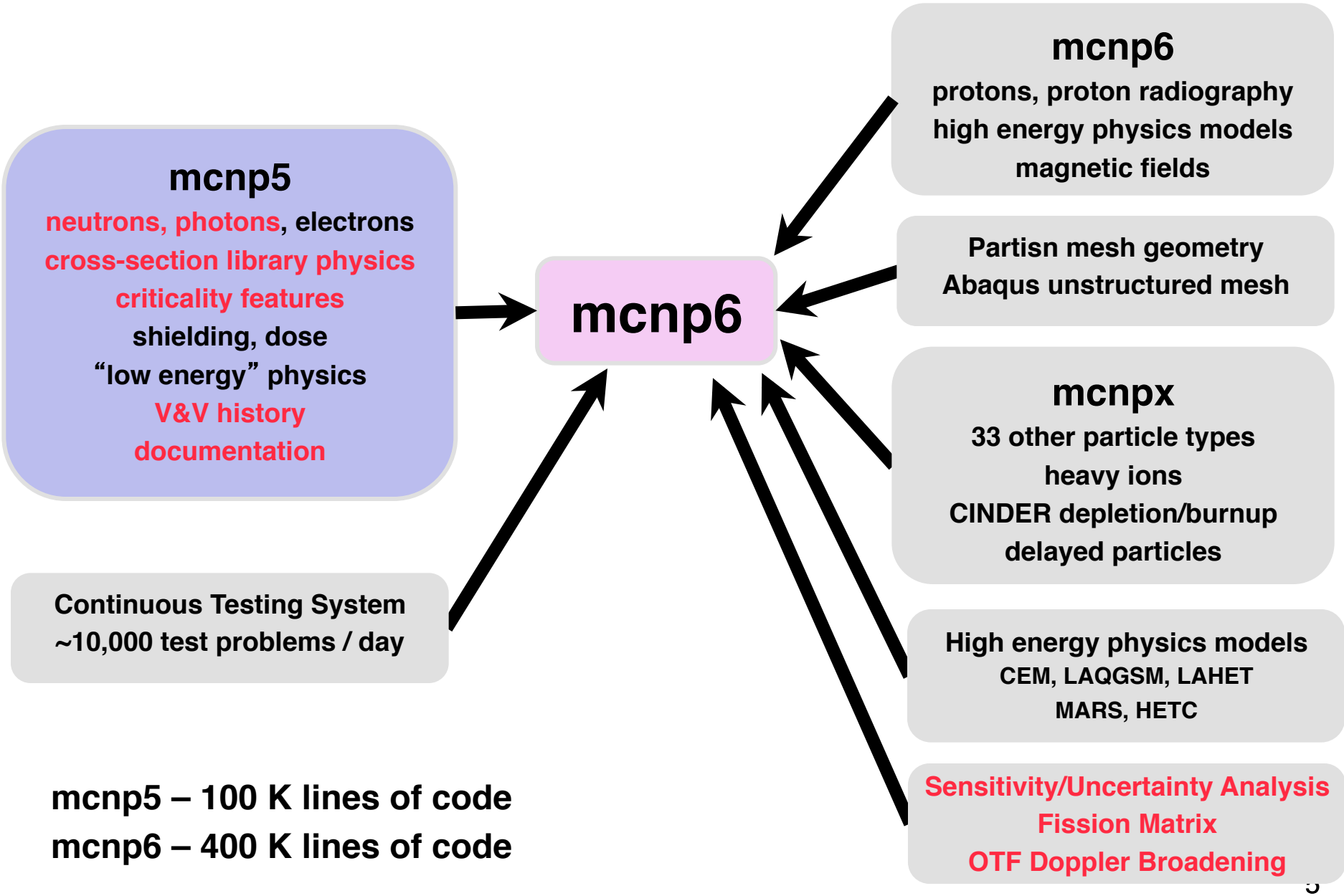
  Nuclear Data Libraries + MCNP Reference Collection

- **MCNP5 & MCNPX are frozen – future development will occur in MCNP6**

Support from DOE/NNSA, DOE, DoD, DRTA, DHS/DNDO, NASA, & others

MCNP5-1.60 vs MCNP6.1

Monte Carlo Codes
XCP-3, LANL



mcnp5 – 100 K lines of code

mcnp6 – 400 K lines of code

MCNP6.1 Release

- **MCNP6.1 = MCNP5 + MCNPX merger**
- **Impact on Criticality Calculations ➜ none**
  - **All KCODE criticality features same as for MCNP5**
  - **Matches results with MCNP5 for criticality suites**
- **Monte Carlo team will support only MCNP6**
- **MCNP6 is here**
  - **Beta-3 release: Jan. 2013**
  - **MCNP6.1: June 2013**
    - Code frozen, V&V and documentation ongoing, installation scripts and DVDs for RSICC being prepared.

Criticality-safety community needs to plan for MCNP5 ➜ MCNP6 transition over the next few years

Verification
&
Validation

Verification / Validation Suites

- **MCNP V&V Suites**

– **VALIDATION_CRITICALITY**	31 ICSBEP experiment benchmarks
– **VALIDATION_CRIT_EXPANDED**	119 ICSBEP experiments
– **CRIT_LANL_SBCS**	194 ICSBEP experiments, from LANL crit-safety group
– **VERIFICATION_KEFF**	75 analytic benchmarks, exact solutions
– **VALIDATION_ROSSI_ALPHA**	Rossi alpha vs experiment
– **VALIDATION_ACODE**	static-alpha eigenvalue benchmarks
– **POINT_KINETICS**	reactor kinetics parameters
– **KOBAYASHI**	void & duct streaming, with point detectors, exact solutions
– **VALIDATION_SHIELDING**	19 shielding/dose experiments
– **REGRESSION**	66 code test problems
– many others for MCNP6	electrons, protons, muons, high-energy physics, delayed particles, magnetic fields, point detectors, MCNP6/Partisn weight window generator, unstructured mesh & ABAQUS linkage, photons, pulse height tallies, string theory models

- **Focus**
  - **Physics-based V&V, compare to experiment or exact analytic results**
  - **Part of MCNP permanent code repository & RSICC distribution**
  - **Automated, easy execution & comparison to experiments**

Current V&V Work

MCNP5-1.51 – 2008
MCNP5-1.60 – 2010
MCNP6-Beta-2 – 2012
MCNP6-Beta-3 – 2013
MCNP6.1 – 2013

- **Detailed V&V for MCNP5 & MCNP6:**

  F.B. Brown, B.C. Kiedrowski, J.S. Bull, "Verification of MCNP5-1.60 and MCNP6.1 for Criticality Safety Applications", LA-UR-13-22196 (2013)

- **Conclusions**
  - **Using the same F90 compiler, MCNP5-1.51, MCNP5-1.60, MCNP6.1 all match results exactly for criticality safety applications**
  - **Switching from Intel-10 to Intel-11/12 introduces some small computer roundoff differences – compiler issue, not code or results**

User Support
&
Training

User Support & Training

- **11,586 copies of MCNP distributed by RSICC, Jan 2001 – Oct 2011**
- **Classes**
  - **Theory & Practice of Criticality Calculations with MCNP5**
    FY12: INL, PNNL/Hanford, LANL, SNL
    FY13: LANL, LANL, **LANL – special class for SB-CS group certification**
  - **Introduction to MCNP5 – classes at LANL**
    FY12: 10/11, 5/12, 6/12
    FY13: 10/29, 5/12, 1/28, 6/3, 6/10
  - **Advanced Variance Reduction – at LANL** 12/3, 8/12
- **Conferences & Journals**
  - ANS San Diego
  - ANS Atlanta
  - M&C 2013
  - NCSD 2013
  - ANS Washington
  - SNA + MC 2013
- **Participated in ANS 10.7 Standards committee**

User Support & Training

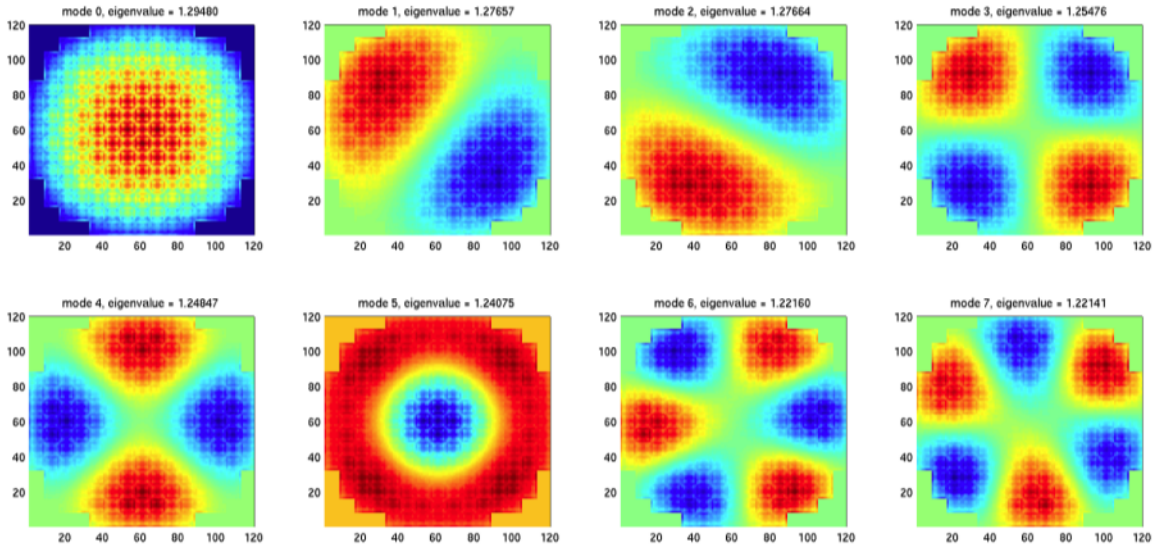
- **MCNP Forum**
  - User-group – beginners & experts, ~1000 members
  - Feedback, bug reports, guidance
- **New MCNP Website**
  - Nice, modern, conforms to LANL requirements
  - Greatly expanded reference collection
- **Reference collection**
  - **1 GB+ of references on Monte Carlo & MCNP**, ~ 600 items
  - Web browser based
  - All MCNP5, MCNP6, & previous MCNP code documentation
  - Criticality, V&V, adjoints, electrons, detectors, parallel, benchmarks, …..
  - Includes 8 half-day Monte Carlo workshops
- **University collaborations**
  - Michigan, New Mexico, Wisconsin, RPI
  - Summer students at LANL

Criticality Related Development

Fission Matrix

Monte Carlo Codes
XCP-3, LANL

- **Obtain higher k-eigenvalues and eigenfunctions**



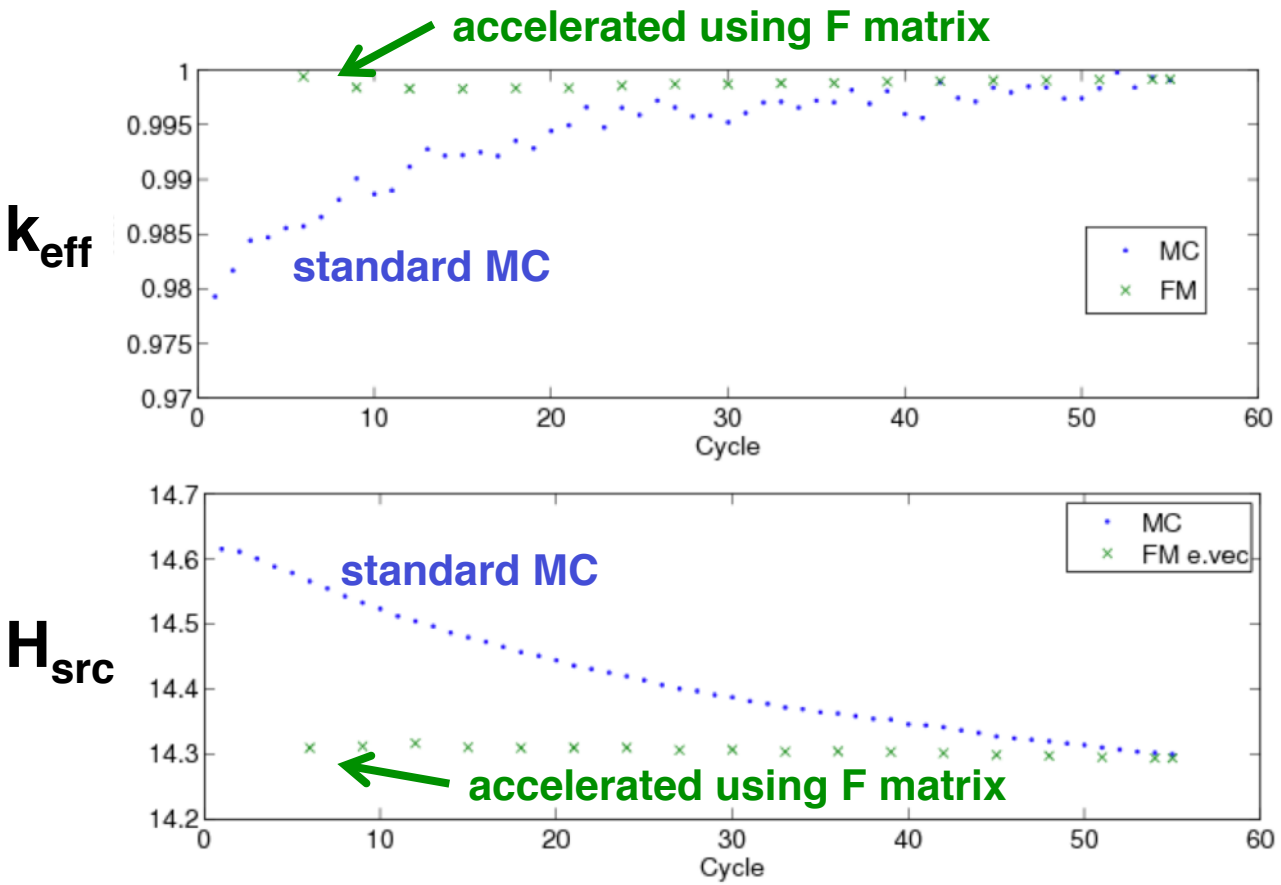
$$S_I = \frac{1}{K} \cdot \sum_{J=1}^{N} F_{I,J} \cdot S_J$$

- **Applications**
  - **Dominance ratio & higher eigenmodes**
  - **Perturbation/transient analysis**
  - **Accelerate convergence, accurate statistical error estimation**

Carney, Brown, Kiedrowski, Martin, "Fission Matrix Capability for MCNP Monte Carlo", Trans ANS 107, San Diego, 2012

- Fission matrix can be used to accelerate convergence of the MCNP neutron source distribution during inactive cycles

- Large increase in convergence rate



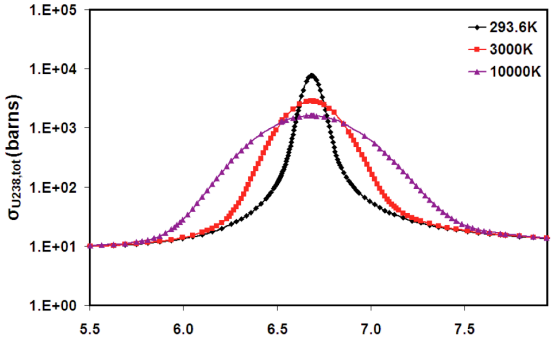
Acceleration using fission matrix for 3D full-core reactor benchmark

On-The-Fly Doppler Broadening

Monte Carlo Codes
XCP-3, LANL

- **Provide general temperature treatment for MCNP**
  - **Continuous temperature capability, without precomputing 1000s of xsec datasets**
  - **Handles an arbitrary number of temperatures**
  - **Necessary for multiphysics: MC + TH + FEM + ...**

- **OTF Methodology (for each nuclide)**
  - **Determine union energy grid for a range of T's**
  - **High-precision fits for σ(E,T) vs T**
  - **MCNP – evaluate σ(E,T) OTF during simulation**
  - 5-10x increase in xsec storage
  - No significant change in cpu time
  - Testing so far – matches explicit precomputed NJOY broadening



- **Current R&D project on temperature coefficients with Univ. of New Mexico.**

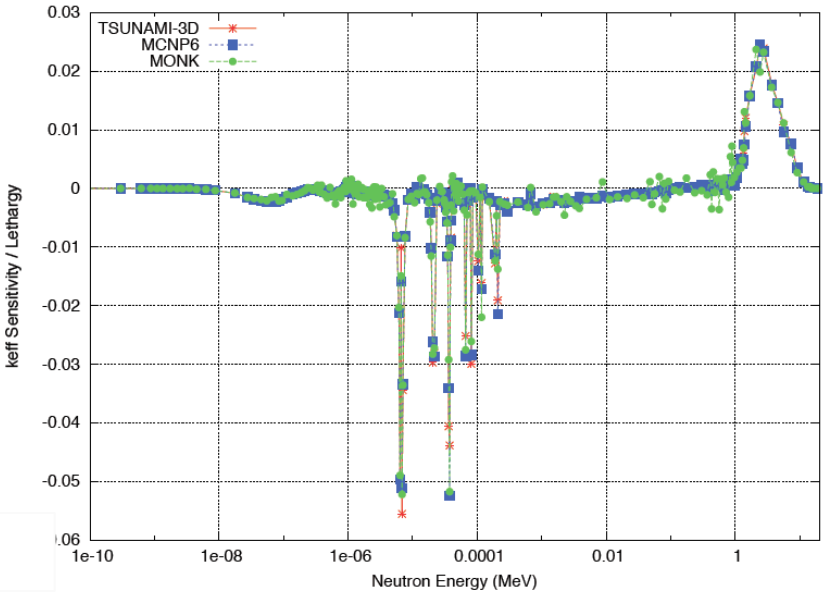
Sensitivity & Uncertainty Progress

Continuous-Energy Sensitivity Coefficients

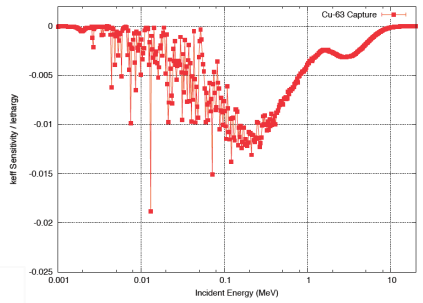
Monte Carlo Codes
XCP-3, LANL

- **MCNP6 can produce sensitivity coefficients to k in continuous-energy**
  - Uses adjoint-weighted perturbations
  - Computes sensitivity coefficients for cross sections, fission, & scattering laws.
  - User-defined energy resolution for results or tallies – no discretization
  - Nuclear Science & Engineering paper accepted and in publication (July 2013)
  - Can directly compare to TSUNAMI multigroup S/U results

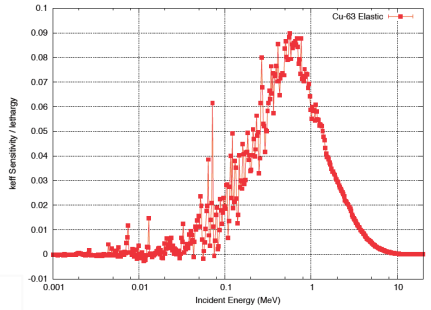
MOX Lattice: U-238 Total



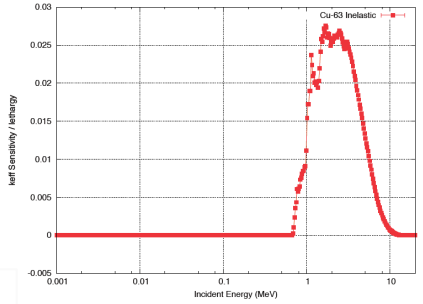
Zeus: Cu-63 Capture Cross-Section Sensitivity



Zeus: Cu-63 Elastic Cross-Section Sensitivity



Zeus: Cu-63 Inelastic Cross-Section Sensitivity



MCNP6 Sensitivity User's Guide on website: LA-UR-13-22251.

ACE Covariance Project

- **Goal: Give MCNP users estimates of uncertainties in keff from nuclear data.**

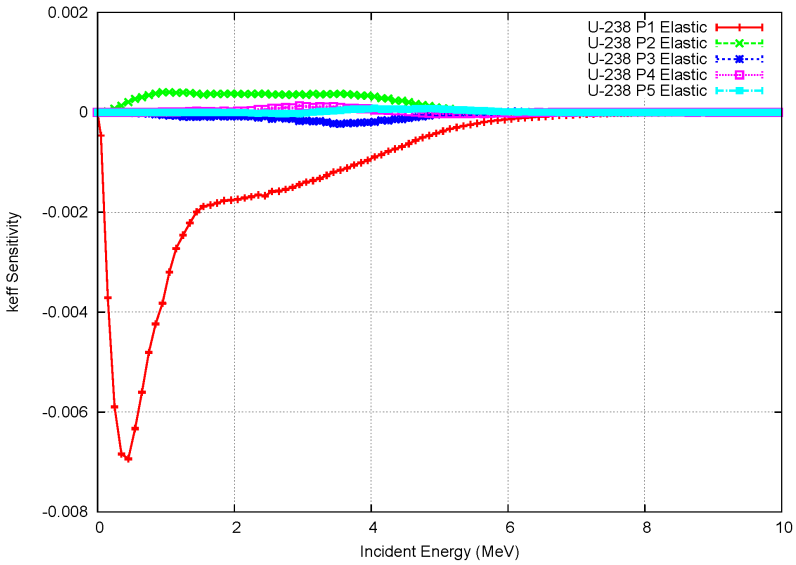
- **Define ACE file format**
  - Uses principal eigenvectors to minimize storage
    - **Kiedrowski, Kahler, Parsions, "Preliminary Covariance Data Representation for the A Compact ENDF File", Trans. Am. Nucl. Soc., 108 (2013).**
    - **Format specifications on MCNP website.**
  - Modifications to NJOY have been proposed
  - To be incorporated into data libraries distributed in MCNP

- **Prototype MCNP version developed that automatically reads in covariance data, produces sensitivity coefficients, and estimates uncertainties.**

- MCNP generated uncertainties (pcm), ENDF/B-VII.1 Pu-239 in Jezebel:

94239.80c	elastic	elastic	462.1
94239.80c	elastic	inelastic	-867.5
94239.80c	elastic	n,2n	-3.4
94239.80c	elastic	fission	-82.2
94239.80c	elastic	n,gamma	36.0
94239.80c	inelastic	inelastic	859.0
94239.80c	inelastic	fission	1.3
94239.80c	n,2n	n,2n	11.1
94239.80c	fission	fission	331.0
94239.80c	fission	n,gamma	0.3
94239.80c	n,gamma	n,gamma	72.4
94239.80c	total nu	total nu	81.6
94239.80c	fission chi	fission chi	174.1
94239.80c			587.6

- **Sensitivities to Legendre moments of angular scattering distributions:**



Flattop U-238 elastic scattering sensitivities. Results show P1 is dominant. Next step is to provide uncertainty estimates from ENDF covariance data.

"K-Eigenvalue Sensitivity Coefficients to Legendre Scattering Moments", LA-UR-13-22431 (submitted to ANS Winter Mtg.)

- **Under development:**
  - **Correlations between isotopes.**
  - **Fixed-source sensitivity capability.**
  - **Extension of eigenvalue sensitivities to more general responses (e.g., reaction rate ratios).**
  - **Temperature coefficients and correlation methods.**

Future of MCNP

MCNP: Challenges of the Near Future

- **MCNP6 has nearly 500k lines of code.**
  - **Old software models unsustainable.**
  - **Very difficult to maintain going forward.**
  - **Changes are necessary and coming!**

- **Path forward involves a concerted effort to modernize the codebase, geared toward modularity and flexibility.**
  - **Necessary for MCNP to survive into the 2020's, otherwise development will become too costly.**
  - **We will require flexibility to continue to take advantage of future hardware architectures -- Can we continue take advantage of Moore's Law?**

Summary and Conclusions

Summary & Conclusions

- MCNP6.1 is here and criticality results have not changed.
  - Users should plan on migrating in the next 1-3 years.

- LANL supports and will continue to support rigorous V&V, testing, user support, and training.

- NCSP funding has led to development of new capabilities in eigenvalue convergence, temperature effects, sensitivity and uncertainty.

- The MCNP development team is preparing to address software development challenges going forward.

Questions ?